



OPPT Chemical Fact Sheets

Butyraldehyde Fact Sheet: Support Document (CAS No. 123-72-8)

This summary is based on information retrieved from a systematic search limited to secondary sources (see Appendix A). These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of butyraldehyde are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF BUTYRALDEHYDE

Characteristic/Property	Data	Reference
CAS No.	123-72-8	
Common Synonyms	butanal	Budavari et al. 1989
Molecular Formula	C ₄ H ₈ O	
Chemical Structure	CH ₃ CH ₂ CH ₂ —CHO	
Physical State	clear, colorless liquid	Keith and Walters 1985
Molecular Weight	72.10	Budavari et al. 1989
Melting Point	-99 °C	Budavari et al. 1989
Boiling Point	74.8 °C	Budavari et al. 1989
Water Solubility	71 g/L @ 25 °C	CHEMFATE 1994
Density	0.802 g/mL	Budavari et al. 1989
Vapor Density (air = 1)	2.48	Verschueren 1983
K _{oc}	9.4 (calculated)	CHEMFATE 1994
Log K _{ow}	0.88 (measured)	CHEMFATE 1994
Vapor Pressure	111.4 mm Hg at 25 °C	CHEMFATE 1994
Reactivity	flammable; reacts with oxidizing materials, acids	Keith and Walters 1985
Flash Point	-6.67 °C (closed cup)	Budavari et al. 1989
Henry's Law Constant	1.15 x 10 ⁻⁴ atm·m ³ /mol	CHEMFATE 1994
Bioconcentration Factor	2.75 (calculated)	CHEMFATE 1994
Odor Threshold	0.0046 ppm	Verschueren 1983
Conversion Factors	1 ppm = 2.9 mg/m ³ 1 mg/m ³ = 0.34 ppm	Verschueren 1983

II. PRODUCTION, USES, AND TRENDS

A. Production

USITC (1994) identified four producers of butyraldehyde in the United States in 1992; TRI92 (1994) identified one additional producer. These five producers are listed in Table 2. In 1992, the U.S. production volume of butyraldehyde was 1,876 million pounds (852,792,000 kilograms; see Table 3). This was a decrease from the 1991 production volume of 1,914 million pounds.

TABLE 2. U.S. PRODUCERS OF BUTYRALDEHYDE AND THEIR CAPACITIES

Producer	Plant Location	1994 Plant Capacity (Millions of Pounds)
Aristech Chemical Company	Pasadena, TX	N/A
BASF Corporation	Freeport, TX	N/A
Eastman Kodak Company, Texas Eastman Company Division	Longview, TX	N/A
Hoechst Celanese Corporation, Chemical Group, Inc.	Bay City, TX	N/A
Union Carbide Corporation, Industrial Chemicals Division	Texas City, TX	N/A

N/A: Not available

Source: USITC (1994); TRI92 (1994)

TABLE 3. U.S. PRODUCTION AND SALES OF BUTYRALDEHYDE

Year	Production (Millions of Pounds)	Sales Quantity (Millions of Pounds)	Sales Value (\$1,000s)	Average Unit Value (Per Pound)
1992	1,876	623	13,714	\$0.21
1991	1,914	695	16,106	\$0.23
1990	1,891	740	16,005	\$0.30
1989	1,679	N/A	N/A	N/A

N/A: Not available

Sources: USITC 1991, 1992, 1993, 1994.

B. Uses

Butyraldehyde is used as an intermediate in the production of synthetic resins, rubber accelerators, solvents, plasticizers, and high molecular weight polymers (Grayson 1985; Sax and Lewis 1987; Windholz 1983). See Table 4 for applicable standard industrial classification (SIC¹) codes.

TABLE 4. END USE PATTERN OF BUTYRALDEHYDE--1992 ESTIMATE

Derivative [Typical Standard Industrial Classification (SIC) Code]	Percentage of U.S. Use
Production of Synthetic Resins (SIC 2821)	N/A
Production of Rubber Accelerators (SIC 2869)	N/A
Production of Solvents (SIC 2869)	N/A
Production of Plasticizers (SIC 2869)	N/A
Production of High Molecular Weight Polymers (SIC 2821)	N/A

N/A: Not Available

Sources: Grayson 1985; Sax and Lewis 1987; Windholz 1983

¹ The Standard Industrial Classification (SIC) code is the statistical classification standard for all Federal economic statistics. The code provides a convenient way to reference economic data on industries of interest to the researcher. SIC codes presented here are not intended to be an exhaustive listing; rather, the codes listed should provide an indication of where a chemical may be likely to be found in commerce.

C. Trends

Demand for butyraldehyde is expected to remain steady for the next few years.

III. ENVIRONMENTAL FATE

A. Environmental Release

Dynamac Corporation (1988) has summarized the occurrence of butyraldehyde in the environment. Butyraldehyde occurs naturally in essential oils of plants and in foods such as fruits, vegetables, cheeses, meat, wines, coffee, honey, and nuts. It has been identified as a metabolite of the poplar tree and as a volatile component of ferns. Butyraldehyde is released to the environment from facilities that manufacture and use it. Exposure in the workplace occurs mainly during sampling, loading and unloading of shipping containers, and maintenance of equipment. Levels as high as 21.3 ppm have been detected for materials-handling workers (8-hour geometric mean time-weighted average, 3.7 ppm). Butyraldehyde has been detected in exhaust emissions from diesel engines (0.08 microliters/L), in gaseous emissions from fireplaces burning jack pine or red oak logs (0.010 to 0.901 g/kg), at hazardous waste sites (an average concentration of 130 ppb in soil, water, and waste samples), and in mother's milk. Urban air samples contained 0.2 to 6 parts per billion (ppb) butyraldehyde. It has also been detected in a surface water sample from the Mississippi River basin and in a marine surface water sample taken from the straits of Florida (22 mg/L).

In 1992, environmental releases of the chemical, as reported to the Toxics Release Inventory by certain types of US industries, totaled about 625,000 pounds, including 496 thousand pounds to the atmosphere, 128 thousand pounds to underground injection sites, 470 pounds to surface water, and 256 pounds to land (TRI92 1994).

B. Transport

Based on one calculation, up to 97% of the butyraldehyde released to any medium would partition to the atmosphere (Dynamac Corporation 1988). However, the vapor pressure (111.4 mm Hg at 25 °C), water solubility (71,000 mg/L), and log K_{ow} value (0.88) for butyraldehyde suggest that the chemical would partition to both air and water (Dynamac Corporation 1988; CHEMFATE 1994). In the atmosphere, butyraldehyde would exist primarily in the vapor phase with a small fraction adsorbed to particulates (HSDB 1994). Its removal from air may occur through wet deposition (HSDB 1994). Butyraldehyde released to water would volatilize with a half-life of about 12 hours, based on its Henry's Law constant (1.15×10^{-4} atm·m³/mol) (CHEMFATE 1994; Dynamac Corporation 1988). Volatilization half-lives of 9 hours and 4.1 days have been estimated for a model river (1 meter deep) and a pond, respectively (HSDB 1994). If released to soil, butyraldehyde will either leach through the soil (K_{oc} of 9.4) or evaporate from soil surfaces (HSDB 1994; CHEMFATE 1994).

C. Transformation/Persistence

1. Air — Butyraldehyde released to the atmosphere is removed primarily by reaction with photochemically-produced hydroxyl radicals (half-life, 16.4 hours) (HSDB 1994). Butyraldehyde may also undergo direct photolysis (HSDB 1994).

2. Water — In water, the major fate processes for butyraldehyde are volatilization (see section III.B) and biodegradation (HSDB 1994). Butyraldehyde is subject to both aerobic and anaerobic biodegradation (Dynamac Corporation 1988). Using various types of inocula, 5-day biological oxygen demand (BOD) values ranging from 28 to 106% have been observed under aerobic conditions (HSDB 1994). Under anaerobic conditions, butyraldehyde was degraded 99% in a Hungate serum bottle (after a 7-day lag period) and 82% in a reactor (after 52 days of acclimation) (Dynamac Corporation 1988; HSDB 1994).
3. Soil — Evaporation, leaching (see section III.B), and biodegradation are the primary fate processes for butyraldehyde in soil (see section III.C.2).
4. Biota — Based on the measured log K_{ow} of 0.88 and the water solubility of 71,000 mg/L for butyraldehyde, the estimated bioconcentration factor (BCF) values are 2.75 and 1.13, respectively, indicating a low potential for bioconcentration in aquatic organisms (HSDB 1994).

IV. HEALTH EFFECTS

A. Pharmacokinetics

1. Absorption — No information was found in the secondary sources searched regarding the absorption of butyraldehyde. Results from toxicity studies presented in Section IV.C suggest absorption of butyraldehyde occurs by the oral and inhalation routes.
2. Distribution — No information was found in the secondary sources searched regarding the distribution of butyraldehyde in the body.
3. Metabolism — Aldehydes, in general, are metabolized to the corresponding acids by the enzyme aldehyde dehydrogenase (Brabec 1981; Dynamac Corporation 1988). This enzyme has been found in every organ of the body that has been studied with the highest activity being in the liver (Dynamac Corporation 1988). The acid metabolite is condensed with coenzyme A and serves as a substrate for fatty acid oxidation and the Krebs cycle (Brabec 1981). Conjugation with glutathione may also occur (Brabec 1981).
4. Excretion — No other information was found regarding the excretion of butyraldehyde; however, glutathione conjugates from similar chemicals have been detected in the urine of experimental animals (Brabec 1981).

B. Acute Effects

Butyraldehyde liquid and vapor damage the eyes and irritate the skin. Generally, the chemical has low acute lethality to laboratory animals.

1. Humans — Human volunteers exposed to butyraldehyde vapor at 230 ppm for 30 minutes reported no eye irritation (Dynamac Corporation 1988). In six cases of industrial corneal injury associated with exposure to butyraldehyde, recovery was rapid and complete (HSDB 1994; Dynamac Corporation 1988). Butyraldehyde liquid is irritating to the skin (HSDB 1994; Dynamac Corporation 1988).
2. Animals — The oral LD_{50} of butyraldehyde in the rat ranges from 2.5 to 5.9 g/kg; the inhalation LC_{50} in the rat is approximately 60,000 ppm (Brabec 1981; Dynamac

Corporation 1988). The chemical is moderately irritating to guinea pig skin and severely irritating to rabbit eyes (Brabec 1981). Bronchial and alveolar edema occurred in rats exposed by inhalation to high levels (not defined) (Brabec 1981). Fatal pulmonary edema has been seen in mice, guinea pigs, and rabbits exposed by inhalation to high levels (Brabec 1981). No signs of toxicity were observed in rats receiving twelve 6-hour inhalation exposures to 1000 ppm (Dynamac Corporation 1988).

C. Subchronic/Chronic Effects

High doses of butyraldehyde administered to animals by oral or inhalation exposure cause lesions of the stomach and respiratory tract, respectively, and decreased body weight.

1. Humans — No information was found in the secondary sources searched regarding the noncarcinogenic subchronic or chronic effects of butyraldehyde in humans.
2. Animals — Male and female rats were treated by gavage with 0, 0.075, 0.15, 0.3, 0.6, or 1.2 g of butyraldehyde/kg 5 days/week for 13 weeks (Dynamac Corporation 1988). In both sexes, a dose-related increase in mortality and a decrease in body weight were observed. There was an increased incidence of irritation, inflammation, necrosis, hyperplasia and lesions of the forestomach and gastric mucosa with 100% of males and 90% of females affected in the high-dose group.

Rats exposed by inhalation to butyraldehyde concentrations of 2710 mg/m³ (934 ppm) for 6 hours/day, 5 days/week, for 20 exposures had oral discharge and increased adrenal and lung weights; no effects were seen at 930 mg/m³ (320 ppm) (U.S. EPA 1989b). Rats and dogs were exposed by inhalation to 0, 125, 500, or 2000 ppm 6 hours/day, 5 days/week for 13 weeks (U.S. EPA 1989a). Rats had mortality (1 animal at 2000 ppm), decreased alkaline phosphatase (500 ppm), altered blood chemistry and decreased red blood cell and monocyte counts (≥ 125 ppm), and lesions of the nasal epithelium and pneumonia (≥ 125 ppm). Dogs had elevated levels of albumin (at 125 ppm) and nasal mucosal lesions (≥ 500 ppm).

Rats, mice, guinea pigs, rabbits, and dogs were exposed by inhalation to 0, 2000, 3100, or 6400 ppm butyraldehyde 6 hours/day, 5 days/week, for 9 days over a 2-week period (U.S. EPA 1989a). Mortality occurred in all species at 6400 ppm; decreased body weights occurred at ≥ 3100 ppm for guinea pigs and mice and at ≥ 2000 ppm for rats; decreased relative kidney and liver weights occurred in rats at ≥ 2000 ppm; and hemorrhage of the ethmoturbinates occurred in one high dose rat.

D. Carcinogenicity

There is insufficient evidence in either humans or animals to classify butyraldehyde as a carcinogen.

1. Humans — An epidemiology study of workers at an acetyl production plant indicated an increase in tumors of the nasal passage, oral cavity, and bronchial airways; however, tumors appeared after relatively short exposure periods and there were multiple chemical exposures (Brabec 1981). In a group of 150 factory workers with more than 20 years of exposure, 9 cases of carcinoma were reported. Multiple aldehydes, including butyraldehyde, and alcohols were detected in the air (Dynamac Corporation 1988).
2. Animals — According to Dynamac Corporation (1988), "plans for a chronic inhalation bioassay of butyraldehyde were dropped by NTP because of technical difficulties in generating the atmosphere for exposure".

E. Genotoxicity

Results from short term mutagenicity testing of butyraldehyde are mixed. Butyraldehyde was negative for mutation in 5 strains of *Salmonella typhimurium* with or without metabolic activation up to 10 mg/plate (HSDB 1994). Butyraldehyde was negative for sister chromatid exchange in human lymphocytes but positive in Chinese hamster ovary cells (<9 mg/mL) (Dynamac Corporation 1988). The chemical was negative for sex-linked recessive lethals in *Drosophila melanogaster* (Dynamac Corporation 1988).

F. Developmental/Reproductive Toxicity

Chromosomal and meiotic anomalies occurred during spermatogenesis in male mice receiving butyraldehyde by either intraperitoneal injection or the drinking water. No information was found on developmental/reproductive effects of butyraldehyde in humans.

1. Humans — No information was found in the secondary sources searched regarding the developmental/reproductive toxicity of butyraldehyde to humans.
2. Animals — Male mice were administered butyraldehyde either in a single intraperitoneal injection of 1 mg/animal or 30 mg/kg or in the drinking water at a concentration of 0.2 mg/L for 50 days (Dynamac Corporation 1988). By either route, chromosomal and meiotic anomalies were observed at all stages of spermatogenesis.

G. Neurotoxicity

Butyraldehyde causes anesthesia in rats at high levels following inhalation exposure.

1. Humans — Due to the distinctive odor and the irritating properties of butyraldehyde, human exposure levels are unlikely to reach concentrations that might induce anesthesia.
2. Animals — Anesthesia occurs in rats exposed by inhalation to high levels (not defined) (Brabec 1981). Dose-responsive reduction in amplitude and decreased conduction velocity were observed in the frog sciatic nerve over the concentration range of 0.01-1.0% butyraldehyde (HSDB 1994).

V. ENVIRONMENTAL EFFECTS

Butyraldehyde is moderately toxic to aquatic species; toxicity values are generally in the range of >1 mg/L to 100 mg/L. Butyraldehyde is not expected to be toxic to aquatic or terrestrial organisms at levels normally found in the environment.

A. Toxicity to Aquatic Organisms

LC₅₀ values for aquatic organisms exposed to butyraldehyde for various durations are as follows: 25.8 mg/L for fathead minnow (*Pimephales promelas*; 96 hours), 114 and 57 mg/L golden orfe (*Leuciscus idus*; two different laboratories, 96 hours), 0.2% (2000 mg/L) for larvae of mosquito (*Aedes aegypti*; 4 hours) (Dynamac Corporation 1988). Minimum inhibitory concentrations of butyraldehyde for various organisms were as follows: 100 mg/L for *Daphnia magna* (based on swimming capability, 24 hours), 100 mg/L for bacterium (*Pseudomonas putida*; based on inhibition of cell multiplication, 24 hours), 4.2 mg/L for flagellate protozoan (*Entosiphon sulcatum*; cell growth, 48 or 72 hours), 98 mg/L for ciliate protozoan (*Uronema parduczi*; cell growth, 48 or 72 hours), and 83 mg/L for green alga (*Scenedesmus quadricauda*; inhibition of cell multiplication, 8 days) (Dynamac Corporation 1988).

B. Toxicity to Terrestrial Organisms

No information was found in the available literature for the toxicity of butyraldehyde in terrestrial species. The oral LD₅₀ values of 2.5 to 5.9 g/kg in laboratory rats suggest that the chemical is acutely toxic to terrestrial animals in very high concentrations.

C. Abiotic Effects

Most butyraldehyde in the atmosphere is removed by reaction with hydroxyl radicals (Dynamac Corporation 1988). According to the definition provided in the Federal Register (1992), butyraldehyde is a volatile organic carbon (VOC) substance. As a VOC butyraldehyde can contribute to the formation of photochemical smog in the presence of other volatile substances.

VI. EPA/OTHER FEDERAL/OTHER GROUP ACTIVITY

The Clean Air Act Amendments of 1990 list butyraldehyde as a hazardous air pollutant. Federal agencies and other groups (listed in Tables 5 and 6) can be contacted for additional information on butyraldehyde.

TABLE 5. EPA OFFICES AND CONTACT NUMBERS FOR INFORMATION ON BUTYRALDEHYDE

EPA Office	Statute	Contact Number
Pollution Prevention & Toxics	PPA ^a	(202) 260-1023
	EPCRA (§313/TRI) ^b	(800) 535-0202
	TSCA (§8A, 8D) ^c	(800) 554-1404
Air	Clean Air Act	(919) 541-0888

^aPPA: Pollution Prevention Act

^bEPCRA: Emergency Planning and Community Right to Know Act of 1986

^cTSCA: Toxic Substances Control Act

TABLE 6. OTHER FEDERAL OFFICES/CONTACT NUMBERS FOR INFORMATION ON BUTYRALDEHYDE

Other Agency/Department/Group	Contact Number
American Industrial Hygiene Association (AIHAWHEEL ^a : 25 ppm [72.5 mg/m ³])	(703) 849-8888
Consumer Product Safety Commission	(301) 504-0994
Food & Drug Administration	(301) 443-3170

^aAIHAWHEEL: American Industrial Hygiene Association Workplace Environmental Exposure Level; an 8-hour TWA (time-weighted-average) is for a normal 8-hour workday and a 40-hour workweek (AIHA 1994).

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APPENDIX A. SOURCES SEARCHED FOR FACT SHEET PREPARATION

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